

## INTERNATIONAL SEARCH REPORT

International Application No  
PCT/EP2005/050778A. CLASSIFICATION OF SUBJECT MATTER  
G06F19/00

According to International Patent Classification (IPC) or to both national classification and IPC

## B. FIELDS SEARCHED

Minimum documentation searched (classification system followed by classification symbols)

G06F

Documentation searched other than minimum documentation to the extent that such documents are included in the fields searched

Electronic data base consulted during the international search (name of data base and, where practical, search terms used)

EPO-Internal, WPI Data, PAJ, BIOSIS, INSPEC, IBM-TDB

## C. DOCUMENTS CONSIDERED TO BE RELEVANT

Category °	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
X	<p>WU Q ET AL: "Empirical correction to density functional theory for van der Waals interactions" JOURNAL OF CHEMICAL PHYSICS, vol. 116, no. 2, 8 January 2002 (2002-01-08), pages 515-524, XP008042179 cited in the application the whole document</p> <p>-----</p> <p>-/-</p>	1-7,15

 Further documents are listed in the continuation of box C. Patent family members are listed in annex.

## ° Special categories of cited documents :

- "A" document defining the general state of the art which is not considered to be of particular relevance
- "E" earlier document but published on or after the international filing date
- "L" document which may throw doubts on priority claim(s) or which is cited to establish the publication date of another citation or other special reason (as specified)
- "O" document referring to an oral disclosure, use, exhibition or other means
- "P" document published prior to the international filing date but later than the priority date claimed

"T" later document published after the international filing date or priority date and not in conflict with the application but cited to understand the principle or theory underlying the invention

"X" document of particular relevance; the claimed invention cannot be considered novel or cannot be considered to involve an inventive step when the document is taken alone

"Y" document of particular relevance; the claimed invention cannot be considered to involve an inventive step when the document is combined with one or more other such documents, such combination being obvious to a person skilled in the art.

"&" document member of the same patent family

Date of the actual completion of the international search

Date of mailing of the international search report

9 September 2005

13-02-2006

Name and mailing address of the ISA

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### Box II Observations where certain claims were found unsearchable (Continuation of item 2 of first sheet)

This International Search Report has not been established in respect of certain claims under Article 17(2)(a) for the following reasons:

1.  Claims Nos.: because they relate to subject matter not required to be searched by this Authority, namely:
  
2.  Claims Nos.: because they relate to parts of the International Application that do not comply with the prescribed requirements to such an extent that no meaningful International Search can be carried out, specifically:
  
3.  Claims Nos.: because they are dependent claims and are not drafted in accordance with the second and third sentences of Rule 6.4(a).

### Box III Observations where unity of invention is lacking (Continuation of item 3 of first sheet)

This International Searching Authority found multiple inventions in this international application, as follows:

see additional sheet

1.  As all required additional search fees were timely paid by the applicant, this International Search Report covers all searchable claims.
  
2.  As all searchable claims could be searched without effort justifying an additional fee, this Authority did not invite payment of any additional fee.
  
3.  As only some of the required additional search fees were timely paid by the applicant, this International Search Report covers only those claims for which fees were paid, specifically claims Nos.:
  
4.  No required additional search fees were timely paid by the applicant. Consequently, this International Search Report is restricted to the invention first mentioned in the claims; it is covered by claims Nos.:

1-9, 11-13, 15

Remark on Protest

The additional search fees were accompanied by the applicant's protest.

No protest accompanied the payment of additional search fees.

**FURTHER INFORMATION CONTINUED FROM PCT/ISA/ 210**

This International Searching Authority found multiple (groups of) inventions in this international application, as follows:

1. claims: 1-9, 11-13, 15

Determining van der Waals parameters for the determination of crystal structures and/or their energies and for the ranking of energies of polymorphic crystal structures.

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2. claims: 10, 14

Numerically optimizing a molecular crystal structure using a crystal coordinate system.

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## C.(Continuation) DOCUMENTS CONSIDERED TO BE RELEVANT

Category °	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
A	<p>PAYNE R S ET AL: "Examples of successful crystal structure prediction: Polymorphs of primidone and progesterone" INTERNATIONAL JOURNAL OF PHARMACEUTICS (AMSTERDAM), vol. 177, no. 2, 25 January 1999 (1999-01-25), pages 231-245, XP002317047 ISSN: 0378-5173 page 231, left-hand column, line 1 - page 232, right-hand column, line 8 page 234, left-hand column, line 17 - page 244, left-hand column, line 7</p> <p>-----</p> <p>KNAPMAN K.: "Polymorphic predictions" MODERN DRUG DISCOVERY, vol. 3, no. 2, March 2000 (2000-03), pages 53-54 AND 57, XP002317048 the whole document</p> <p>-----</p> <p>VERWER P ET AL: "COMPUTER SIMULATION TO PREDICT POSSIBLE CRYSTAL POLYMORPHS" REVIEWS IN COMPUTATIONAL CHEMISTRY, VCH, NEW YORK, NY, US, vol. 12, October 1998 (1998-10), pages 327-365, XP008042156 ISSN: 1069-3599 the whole document</p> <p>-----</p> <p>NEUMANN M A ET AL: "Recent advances in structure solution from powder diffraction data" INTERNATIONAL JOURNAL OF MODERN PHYSICS B WORLD SCIENTIFIC SINGAPORE, vol. 16, no. 1-2, 2002, pages 407-414, XP008042435 ISSN: 0217-9792 abstract page 413, line 5 - page 414, line 2</p> <p>-----</p>	8,9, 11-13,15
A		8,9, 11-13,15
A		
A		